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Electromigration theory unified

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Abstract. – The starting formula of Bosvieux and Friedel (*J. Phys. Chem. Solids*, **23** (1962) 123) for the force on an ion in a metal due to an applied voltage is shown to lead to the same description as the linear-response approach used in the field since its introduction by Kumar and Sorbello (*Thin Solid Films*, **25** (1975) 25). By this electromigration theory has become a unified theory. This follows after accounting for a treacherous trap term, which at first sight seems to be zero. Up to now, Bosvieux and Friedel claimed to predict a completely screened direct force, which means that only a wind force would be operative. In addition, the amount of screening has been calculated up to second order in the potential of the migrating impurity, using a finite temperature version of the screening term derived by Sham (*Phys. Rev. B*, **12** (1975) 3142). For a proton in a metal modeled as a jellium the screening appears to be about 15%, which is neither negligible nor reconcilable with the old full-screening point of view.

Introduction. – Electromigration is the motion of an ion in a metal under the influence of an applied voltage. Depending on the metal and the ion, its motion is either to the anode or to the cathode. The total driving force \mathbf{F} on such an ion is known to be the result of two contributions, a direct force and a wind force:

$$\mathbf{F} = \mathbf{F}_{direct} + \mathbf{F}_{wind} = (Z_{direct} + Z_{wind})e\mathbf{E} = Z^*e\mathbf{E}, \quad (1)$$

in which Z^* is called the effective valence, which is a measurable quantity. The direct force is due to the direct action of the applied field \mathbf{E} on the charge of the ion. The wind force comes from the scattering of the current carrying electrons off the ion [1].

Until 1962 there was a common belief that Z_{direct} was equal to the bare valence Z_i of the ion. At most a small deviation from that value could arise from the electrons in the metallic environment of the ion. In 1962 Bosvieux and Friedel [2] predicted a complete cancellation of the direct force due to screening effects, so that only the wind force would remain. By that prediction a controversy was born. It was not easy to decide matters by a measurement, and a satisfactory theoretical answer was lacking as well.

In 1975 Kumar and Sorbello [3] published an exact linear-response expression for the driving force. After that it was considered as being just a matter of a careful evaluation of that expression in order to settle the problem. It took quite some time to do so though. Finally

Sorbello [4], starting from the complicated treatment given by Rimbey *et al.* [5], predicted a screening of 10–30%, depending on the potential used for the ion. Support of this result has been given by the present author, starting from a much simpler description [6]. However, in the meantime new support was given for the full-screening point of view [7].

Interestingly, the original paper by Bosvieux and Friedel (BF) is referred to as being controversial on the one hand, while on the other hand their starting formula is referred to as the first quantum-mechanical equation for the wind force, which is seen as a pioneering contribution to the field. Therefore we undertook an new evaluation of their starting formula, following the authors as closely as possible, up to a point where we came across a trap. By treating this trap properly the final evaluation ends up at the standard linear-response expression for the driving force. As far as the author knows, Sorbello was the first who showed that such traps occur in the theory of electromigration [8].

The screening itself has been calculated by Sorbello [4], who used one type of expression for it. Therefore we undertook the evaluation of Sham's second-order expression written in a new form, the more so as a more recent result for the screening, ranging from 0 to 100%, is rather inconclusive [9]. Sham's expression has never been evaluated numerically, and in his paper he just gives an order of magnitude comparison with his wind force expression [10]. This has led him to the conclusion that the screening is negligible. We find a screening of 5–25%, which is in agreement with Sorbello's results.

Rydberg atomic units are used, in which the energy is in rydberg, the distance is in bohr (1 bohr $\approx 0.5 \text{ \AA}$), $\hbar = 1$, and the electronic mass is $\frac{1}{2}$.

Basics of linear-response theory. – We first give the standard linear-response expression for the driving force on an ion at position \mathbf{R}_i [11],

$$\mathbf{F} = Z_i e \mathbf{E} - ie E_\nu \int_0^\infty dt e^{-at} \text{Tr} \left\{ \rho(H) \left[\mathbf{F}_{\text{op}}(t), \sum_j r_j^\nu \right] \right\}, \quad (2)$$

in which the Cartesian label ν runs from 1 to 3. The infinitesimally positive number a represents the adiabatical switch-on of the electric field, the operator $\rho(H)$ is the grand-canonical density depending on the system Hamiltonian H , the force operator \mathbf{F}_{op} stands for

$$\mathbf{F}_{\text{op}} \equiv -\nabla_{\mathbf{R}_i} V = -\sum_j \nabla_{\mathbf{R}_i} v(\mathbf{r}_j - \mathbf{R}_i) \equiv \sum_j \mathbf{f}_j^i, \quad (3)$$

and its time dependence refers to the Heisenberg representation $\mathbf{F}_{\text{op}}(t) \equiv e^{iHt} \mathbf{F}_{\text{op}} e^{-iHt}$. The expression published by Kumar and Sorbello [3] follows simply after a partial integration in eq. (2) with respect to the time.

All important studies of the driving force have been done for the electron-impurity system, the Hamiltonian H of which can be written as a sum of single-particle Hamiltonians h , so $H = \sum_j h^j$ with $h = h_0 + v = h_0 + \sum_\alpha v^\alpha$. The summation in the electron-impurity potential v runs over the positions \mathbf{R}_α of the impurities. This allows for a reduction of the many-body expression (2) to the following single-particle expression:

$$\mathbf{F} = Z_i e \mathbf{E} - ie E_\nu \int_0^\infty dt e^{-at} \text{tr} \left\{ n(h) [\mathbf{f}^i(t), r^\nu] \right\}, \quad (4)$$

where $n(h)$ is the Fermi-Dirac distribution function in operator form

$$n(h) = \frac{1}{e^{\beta(h - \epsilon_F)} + 1}. \quad (5)$$

The treatment of Bosvieux and Friedel (BF). – We start to follow BF's treatment, by writing down their system Hamiltonian

$$H = - \sum_{\mu=1}^N \frac{\Delta_{\mu}}{2m_{\mu}} + V(\mathbf{r}_1, \dots, \mathbf{r}_{\mu}, \dots, \mathbf{r}_N). \quad (6)$$

In applying a small perturbation denoted as δV they write down the perturbed wave function Ψ . In their appendix BF employ the idea of switching on the field adiabatically. For the sake of clarity we give the explicit form of the perturbing potential due to an applied field,

$$\delta V(t) = e\mathbf{E}e^{at} \cdot \left(\sum_j \mathbf{r}_j - \sum_{\alpha} Z_{\alpha} \mathbf{R}_{\alpha} \right) \equiv \delta V e^{at} \equiv (\delta V(\mathbf{r}) + \delta V(\mathbf{R}))e^{at}, \quad (7)$$

which is zero in the limit $t \rightarrow -\infty$. The position-dependent potentials have been defined for later use. BF's force expression reads as

$$\vec{\phi} = -\langle \Psi | \nabla_i (V + \delta V) | \Psi \rangle, \quad (8)$$

in which $|\Psi\rangle$ represents the state of the system as it develops from its unperturbed ground state $|\psi_0\rangle$ due to the perturbation δV . In order to find $|\Psi\rangle$ we solve the time-dependent Schrödinger equation

$$i \frac{\partial \Psi(t)}{\partial t} = \mathcal{H}(t) \Psi(t) \quad (9)$$

for the total Hamiltonian $\mathcal{H}(t) = H + \delta V(t)$ by working in the interaction representation for $\Psi(t)$, defined as $\Psi_I(t) \equiv e^{iHt} \Psi(t)$. Using eq. (9), one finds straightforwardly that the time derivative of $\Psi_I(t)$ is equal to $-ie^{iHt} \delta V(t) e^{-iHt} \Psi_I(t)$. Integration of this equation leads to the following expression for $\Psi(t)$ linearly in δV :

$$\Psi(t) = -ie^{-iHt} \int_{-\infty}^t dt' e^{iHt'} \delta V(t') e^{-iHt'} \Psi_I(-\infty) + e^{-iHt} \Psi_I(-\infty). \quad (10)$$

With $\delta V(t) = \delta V e^{at}$, applying the substitution $t - t' \equiv s$, and considering an arbitrary time in the present, so $t = 0$, this becomes

$$\Psi(0) \equiv \Psi = -i \int_0^{\infty} dt e^{-(iH+a)t} \delta V e^{iHt} \Psi_I(-\infty) + \Psi_I(-\infty). \quad (11)$$

If one calculates matrix elements with this $|\Psi\rangle$ the factor $e^{-iE_0\infty}$ in the state $|\Psi_I(-\infty)\rangle$ drops out so that just the ground state $|\psi_0\rangle$ remains. BF's eq. (I.2) for $|\Psi\rangle$ is reproduced by inserting the complete set of eigenstates of the system Hamiltonian H , denoted by $|\psi_n\rangle$. The only difference is the presence of the infinitesimal number a . BF have put $a = 0$ and just restrict the summation over n to all values $n \neq 0$. It will become clear that this difference has a dramatic influence on the final results.

Now we evaluate BF's force expression, eq. (8), linearly in the applied field δV :

$$\begin{aligned} \vec{\phi} &= -\langle \psi_0 | \nabla_i (\delta V) | \psi_0 \rangle + i \int_0^{\infty} dt e^{-at} \langle \psi_0 | (\nabla_i V) e^{-iHt} \delta V e^{iHt} | \psi_0 \rangle + \text{c.c.} \\ &= Z_i e \mathbf{E} + i \int_0^{\infty} dt e^{-at} \langle \psi_0 | \left[(\nabla_i V), e^{-iHt} \delta V e^{iHt} \right] | \psi_0 \rangle, \end{aligned} \quad (12)$$

in which we used eq. (7) for evaluating the matrix element $\langle \psi_0 | \nabla_i (\delta V) | \psi_0 \rangle$.

In the further evaluation of this equation we want to follow BF's evaluation given in their §I. The integral in the first line of eq. (12) is carried out after inserting the complete set $|\psi_n\rangle$. Using the equality $(\nabla_i V) = [\nabla_i, H]$ one obtains

$$\begin{aligned}\vec{\phi} &= Z_i e \mathbf{E} - \sum_n (E_n - E_0) \langle \psi_0 | \nabla_i | \psi_n \rangle \frac{\langle \psi_n | \delta V | \psi_0 \rangle}{E_0 - E_n + ia} + \text{c.c.} \\ &= Z_i e \mathbf{E} + \langle \psi_0 | \nabla_i \delta V | \psi_0 \rangle - ia \sum_n \langle \psi_0 | \nabla_i | \psi_n \rangle \frac{\langle \psi_n | \delta V | \psi_0 \rangle}{E_0 - E_n + ia} + \text{c.c.} \\ &= -ia \sum_n \langle \psi_0 | \nabla_i | \psi_n \rangle \frac{\langle \psi_n | \delta V | \psi_0 \rangle}{E_0 - E_n + ia} + \text{c.c.}\end{aligned}\quad (13)$$

The second line is obtained after the replacement $E_n - E_0 \rightarrow E_n - E_0 - ia + ia$ and carrying out the sum over n for the first term. We want to comment on eq. (13) in view of the results of BF. First, in evaluating the matrix element $\langle \psi_0 | [\nabla_i, H] | \psi_n \rangle$ in the first line of eq. (13), BF create in addition surface integral terms corresponding to Green's theorem, by that not appreciating the Hermitian property of H . These surface integral terms represent flow of probability out of the system, which is obviously zero for a finite system and for an isolated metal, as BF admit. But this flow is zero also for a metal carrying a steady electric current, which is denied in practice by BF. Secondly, in their treatment the last line of eq. (13) is missing, because BF have $a = 0$. We want to point out that regarding this last line a treacherous trap in the formalism is involved, which has shown up earlier in electromigration theory [8]. This term seems to be zero because of the proportionality with the infinitesimal number a , but we will show that this term in fact is a rich one.

In rewriting the last line of eq. (13) we write the energy denominator as a time integral, after which the summation over n can be carried out. One finds

$$\vec{\phi} = -a \int_0^\infty dt e^{-at} \langle \psi_0 | [\nabla_i, e^{-iHt} (\delta V(\mathbf{r}) + \delta V(\mathbf{R})) e^{iHt}] | \psi_0 \rangle, \quad (14)$$

in which δV has been replaced by the two position-dependent terms according to eq. (7). Because H commutes with $\delta V(\mathbf{R})$, the second term reduces to $Z_i e \mathbf{E}$, and one finds that

$$\vec{\phi} = Z_i e \mathbf{E} - a \int_0^\infty dt e^{-at} \langle \psi_0 | [e^{iHt} \nabla_i e^{-iHt}, \delta V(\mathbf{r})] | \psi_0 \rangle. \quad (15)$$

After a partial integration with respect to time, using that $[\nabla_i, H] = (\nabla_i V)$, and substituting $\delta V(\mathbf{r})$ according to eq. (7), one finds

$$\vec{\phi} = Z_i e \mathbf{E} + i \int_0^\infty dt e^{-at} \langle \psi_0 | [e^{iHt} (\nabla_i V) e^{-iHt}, e \mathbf{E} \cdot \sum_j \mathbf{r}_j] | \psi_0 \rangle. \quad (16)$$

We are back at the second line of eq. (12), but only the electron coordinates in δV have survived the operations. The influence of the electric current on the total force is taken care of by the second term in the right-hand side of eq. (16). In retrospect this result follows rightaway from eq. (12) as well, but we wanted to go along with BF's way of evaluation first.

Equation (16) is a very interesting result. It is precisely the zero-temperature equivalent of eq. (2). This becomes even clearer if we write down the form which shows up after the reduction of eq. (16) to single-particle states denoted by $|q\rangle$,

$$\vec{\phi} = Z_i e \mathbf{E} + i \int_0^\infty dt e^{-at} \sum_q \langle q | [e^{iht} (\nabla_i v) e^{-iht}, e \mathbf{E} \cdot \mathbf{r}] | q \rangle. \quad (17)$$

At $T = 0$ the sum over the single-particle states has a sharp cut-off at $\epsilon_q = \epsilon_F$. The finite-temperature equivalent of eq. (17) can be written as

$$\begin{aligned}\vec{\phi} &= Z_i e \mathbf{E} + i \int_0^\infty dt e^{-at} \sum_q n(\epsilon_q) \langle q | \left[e^{iht} (\nabla_i v) e^{-iht}, e \mathbf{E} \cdot \mathbf{r} \right] | q \rangle \\ &= Z_i e \mathbf{E} - i \int_0^\infty dt e^{-at} \text{tr} \left\{ n(h) \left[\mathbf{f}^i(t), e \mathbf{E} \cdot \mathbf{r} \right] \right\} \equiv (Z_i + Z_{wind} + Z^{scr}) e \mathbf{E},\end{aligned}\quad (18)$$

in which the Fermi-Dirac distribution $n(\epsilon)$ has been inserted, see eq. (5). The force operator \mathbf{f}^i is defined in eq. (3). Clearly, eq. (18) is completely equivalent to eq. (4) of the present text. By this electromigration theory can be considered as being unified. Apparently, BF's starting formula was correct, but these authors did not recognize its precise contents. This became even clearer recently [12]. BF used eq. (8) for their result regarding the direct force only. They treated the wind force separately, applying a semi-classical standard approach in describing the current-carrying electrons and accounting for the scattering of the electrons by the migrating impurity quantum-mechanically [13].

The formal eqs. (2) or (18), or forms which have been shown to be equivalent to them, have been used since Kumar and Sorbello published their linear-response approach to the electromigration problem [3]. The result of all this research is that the second term of these equations contains two contributions, as has been indicated explicitly in the right-hand side of eq. (18). One can be identified as the wind force. The other one implies some screening of the bare direct force $Z_i e \mathbf{E}$. The wind force expression has been studied thoroughly [14, 15]. Because the present paper is devoted to the settlement of the controversy regarding the direct force, we want to add a calculation of Z^{scr} starting from Sham's contribution [10]. But first one more comment on eq. (18) and its interpretation. BF claim to have proven that for an isolated system the force on an ion is zero [12]. The present author agrees that this force is zero, but this fact does not follow from an explicit proof, but from the knowledge that internally any applied field \mathbf{E} is screened out by an electronic surface charge that is built up. This is a general result from the theory of electromagnetism. That is why then $\vec{\phi}$, which is proportional to \mathbf{E} , is zero, because $\mathbf{E} = 0$.

Calculation of Z^{scr} . – If one evaluates eq. (18) to lowest order in the potential v of the ion, for a jellium model of the metal, one finds that [16]

$$Z^{scr} = -\frac{4}{3m} \sum_{kk'} (k^2 - \mathbf{k} \cdot \mathbf{k}') \frac{|v_{kk'}|^2}{(\epsilon_k - \epsilon_{k'})^2 + a^2} \left(\frac{\partial n_k}{\partial \epsilon_k} - \frac{n_k - n_{k'}}{\epsilon_k - \epsilon_{k'}} \right), \quad (19)$$

in which a k label refers to a plane wave. It has been shown that the $T \rightarrow 0$ limit is equivalent to Sham's expression [16]. Sham gave an order of magnitude estimate by comparing it with the wind force expression. Z_{wind} is proportional to the transport relaxation time τ of the system, while Z^{scr} is proportional to the inverse of an energy, for which the Fermi energy can be chosen. By that he came out at a ratio of $(\epsilon_F \tau)^{-1} \approx 0.01$, being negligible.

A numerical evaluation of Z^{scr} becomes possible if one employs the spherical wave expansion for a plane wave, converts the summations over the wave vectors to integrals and carries out the angular integrals over the directions of the wave vectors. After using the relation between k^2 and the energy ϵ_k one ends up at

$$Z^{scr} = -\frac{4}{3\pi^2 m} \int_0^\infty d\epsilon_k \int_0^\infty d\epsilon_{k'} \frac{\frac{\partial n_k}{\partial \epsilon_k} - \frac{n_k - n_{k'}}{\epsilon_k - \epsilon_{k'}}}{(\epsilon_k - \epsilon_{k'})^2 + a^2} \sum_\ell f_\ell(k, k'), \quad (20)$$

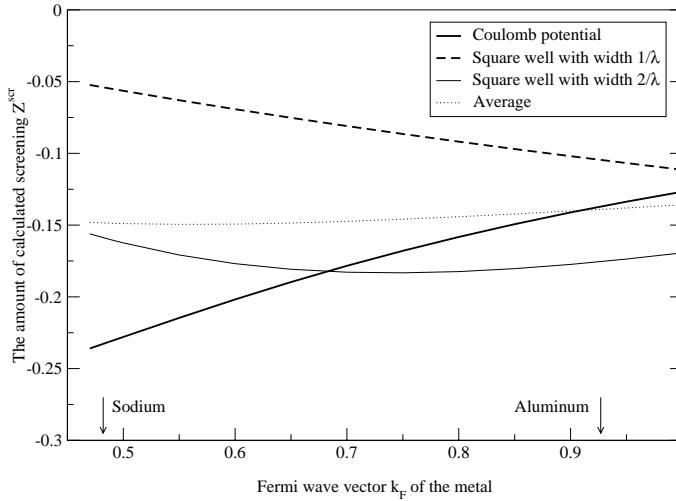


Fig. 1 – The amount of screening represented by Z^{scr} according to eq. (20), with $a = \tau^{-1}$ and $\tau = 100$, for the screened Coulomb potential and for two square-well potentials.

in which the function $f_\ell(k, k')$ is defined as

$$f_\ell(k, k') = \epsilon_k \sqrt{\epsilon_{k'}} v_\ell(k', k) \left[(2\ell + 1)k v_\ell(k', k) - 2(\ell + 1)k' v_{\ell+1}(k', k) \right], \quad (21)$$

containing the information about the ion potential through

$$v_\ell(k', k) = \int_0^\infty r^2 dr j_\ell(k'r) v(r) j_\ell(kr). \quad (22)$$

The integrand has to be treated with care when $\epsilon_{k'} = \epsilon_k$, because then the denominator attains the value a^2 which would imply “singular” behaviour. However, precisely then the numerator becomes zero, because $\lim_{\epsilon_{k'} \rightarrow \epsilon_k} (n_k - n_{k'}) / (\epsilon_k - \epsilon_{k'}) \rightarrow \frac{\partial n_k}{\partial \epsilon_k}$. The crucial part of the integrand lies in the square around the point $(\epsilon_k, \epsilon_{k'}) = (\epsilon_F, \epsilon_F)$. In studying the Z^{scr} integral it appears that in that square one has to keep the Fermi-Dirac distribution function in its finite-temperature form. A calculation for $a \ll \tau^{-1}$ has been presented elsewhere [17]. Here we want to follow Sham more closely. He replaced a by τ^{-1} , by that accounting for all possible dissipation mechanisms.

The result of a numerical evaluation for different ion potentials is shown in fig. 1. In addition to a screened Coulomb potential $v(r) = -Z_i e^2 e^{-\lambda r} / r$ [13], with the Thomas-Fermi screening parameter λ , square-well potentials were employed in the same spirit as Sorbello did [4]. The choice $Z_i = 1$ represents a proton in a jellium. The width of the square-well potential was chosen to be equal to the screening length $1/\lambda$ and twice as large. The corresponding well depth was limited by the condition that just no bound state could be formed. The value of λ is determined by the Fermi energy. While Sorbello chose five values for the Fermi energy, typical for metals ranging from sodium to aluminum, we have done the calculation for a whole range of Fermi energies. The results are plotted as a function of the Fermi wave number k_F . The k_F values of sodium and aluminum are indicated.

Because λ increases monotonically with the Fermi energy, the range of the corresponding screened Coulomb potential decreases with increasing k_F , whose reduction in strength is seen

clearly in the bold solid curve. We compared v_{kk} for the three potentials and found a clear decrease for the Coulomb potential with increasing k_F , and a rather flat behaviour for the square-well potentials, the one with $2/\lambda$ being markedly stronger than the one with the smaller width. The screening to second order in the impurity potential appears to be not negligible, but on the average equal to $15 \pm 10\%$. As a guide for the eye we gave the average of Z^{scr} for the three potentials as a dotted line. Interestingly, this result does not imply that Sham's conclusion of a negligible screening is entirely wrong. In fact, he compared Z^{scr} with Z_{wind} . The ratio Z^{scr}/Z_{wind} is small indeed, but this comes from the large value of τ . It may be clear that a comparison with Z_i would have been more appropriate.

In conclusion, we have shown that the starting formula of Bosvieux and Friedel gives the right driving force on an ion in a metal under the influence of an applied voltage. Because it always has been recognized as the first time that a quantum-mechanical formula for that force was written down, their contribution can still be characterized as a pioneering one. On the other hand, their prediction of a complete cancellation of the direct force has been falsified, because it was based on surface integral terms, which are zero due to the hermiticity of the system Hamiltonian. Further, the expression for the magnitude of the screening due to Sham does not give a negligible screening, but a screening of about 15%. This is in agreement with an earlier result based on another approach [4].

Taking all this together, the controversy regarding the direct force can be regarded as being resolved by now, and a unification of the various descriptions has been achieved.

* * *

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